09.2-3 CRYSTAL STRUCTURE OF 1-(5-CARBOMETHOXY-2-FURYL)-2,2,2-TRICHLOROETHANOL. By F. Pajaro and R. Ponce, University of Oriente and Academy of Science of Cuba, Santiago de Cuba, Cuba.

C₇H₉O₂Cl₃, orthorhombic, space group Pbcn, a = 18.00(1), b = 13.72(1), c = 7.13(1)Å, β = 90°, 406 F(hkl) were refined.

A three-dimensional data set was collected at room temperature with MoKa radiation (λ = 0.7093 Å), using a perpendicular beam diffractometer with a graphite monochromator. Data were recorded by the ω-2θ scan technique to a maximum 2θ value of 48°. The structure was solved by direct methods. The coordinates and the anisotropic temperature factors for the non-hydrogen atoms were refined by full-matrix least-squares methods to a final R value 0.046.

![Molecular structure of C₇H₉O₂Cl₃](image)


The structure and conformation of the triaccharide, mannotriose, are reported. The crystal structure space group is F21, a = 11.834(2), b = 12.27(1), c = 9.123(2), β = 112.34(2), solved by using SHELX and refined using SHELX, with anisotropic scale factors, from 1769 reflections with D3(01). Final R = 0.048 with unit weights. The conformation of the molecule is stabilised by intra-molecular hydrogen bonds 0(13)-0(5) and 0(13)-0(13). Each molecule is extended, has its long axis at about 45° to the c and b axes, and is approximately perpendicular to the c axis, producing a pattern which resembles a herring-bone brick bond. Water molecules in the interstices take part in hydrogen bonds reinforcing the inter-layer connections.

The central residue, with torsion angles ϕ(1) = -84.3°, ϕ(4) = -169.0°, ϕ(2) = -73.2° and ϕ(2) = -132.17° provides a good model for a poly(1→4)mannoside, c.f. β-cellotriose undecasaccharate (Perez, S. & Bisse, P. Acta Cryst. (1977) B33, 2578-2584) for a poly(1→4) glucoside.

09.2-6 CRYSTAL AND MOLECULAR STRUCTURE OF 1,2,3,4,5,6,7,8-Octahydro-7-anthryl-1-β-[N-methyl-2-β-[O-acetyl-o-glucopyranosyl(1→2) β-gluco-8-mannosyl(1→3)]-3,4,9,10,11,12-hydrophenanthrene(11/4O)]. By B. Chatterjee, Physics Department, Visva-Bharati University, Santiniketan-731235, West Bengal, India.

The presence of partially aromatised hydrocarbons related to steroids has been noticed in geological samples and the first identification of one type has been reported (J. Schaeffle et al., Tetrahedron Lett., 1976, 4153). In connection with the total synthesis of this partially aromatised hydrocarbon and related compounds a stereospecific CM-reduction of a hydrophenanthrene derivative yielded the title compound, an A/B CD Ketone, as an intermediate (J. Schaeffer et al., J. Chem. Soc., Chem. Commun., 1982, 84).

![Figure. Cyclophosphamidines.](image)

It is suggested that compounds having this type of A/B CM-configuration with a ring fusion methyl group and a ring fusion hydroxyl, usually equilibrate between the two canonical conformers owing to their flexible nature. An X-ray diffraction study of this Ketone has been undertaken to confirm the stereospecifity of the CM reduction.